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(54) Title: CRYSTAL STRUCTURE OF CHORISMATE SYNTHASE AND USES THEREOF

(57) Abstract: The invention describes the identification of the struc-
ture coordinates for the enzyme Chorismate Synthase. There is a com-
puter programmed to produce a three-dimensional representation of a
molecule or molecular complex, wherein the molecule or molecular
complex comprises a binding domain defined by the structure coordi-
nates of (a) Arg 39, His 110, Ser 132, Thr 136, Lys 254, Gly 297, Lys
311, Thr 315, Arg 337 and Asp 339 ; or (b) Ser 9, His 10, Arg 39, Asp
54, Arg 107, His 110, Ser 132, Ala 133, Arg 134, Thr 136, Arg 337 and
Asp 339. 1, or where the molecular complex or binding domain has
a root mean square deviation of conserved residue backbone atoms of
less than 2A when superimposed on the relevant backbone atoms de-
scribed by the structure coordinates of said amino acids.

ATOM	119	CA	GLY A	20	-10.000	-2.288	-9.535	1.00	21.18	6	A	C
ATOM	120	C	GLY A	20	-9.253	-2.448	-8.716	1.00	20.63	6	A	C
ATOM	121	O	GLY A	20	-8.353	-2.753	-8.824	1.00	20.20	6	A	C
ATOM	122	H	GLY A	20	-10.318	-2.922	-8.000	1.00	18.32	6	A	C
ATOM	123	CA	ILE A	21	-9.813	-6.431	-7.327	1.00	19.14	6	A	C
ATOM	124	C	ILE A	21	-9.493	-7.259	-6.432	1.00	20.03	6	A	C
ATOM	125	O	ILE A	21	-10.493	-7.259	-6.432	1.00	19.14	6	A	C
ATOM	126	CB	ILE A	21	-10.978	-6.803	-6.255	1.00	20.46	6	A	C
ATOM	127	CG	ILE A	21	-10.764	-6.719	-6.258	1.00	19.51	6	A	C
ATOM	128	CD	ILE A	21	-10.764	-6.719	-6.258	1.00	19.51	6	A	C
ATOM	129	CE	ILE A	21	-9.749	-5.697	-7.285	1.00	17.88	6	A	C
ATOM	130	CGA	ILE A	21	-9.749	-5.697	-7.285	1.00	17.88	6	A	C
ATOM	131	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	132	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	133	CA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	134	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	135	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	136	CB	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	137	CG	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	138	CD	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	139	CE	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	140	CF	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	141	CGA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	142	C	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	143	O	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	144	CA	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	145	C	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	146	O	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	147	CB	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	148	CG	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	149	CD	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	150	CE	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	151	CF	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	152	CGA	ALA A	23	-11.453	-2.214	-10.068	1.00	18.82	6	A	C
ATOM	153	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	154	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	155	CA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	156	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	157	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	158	CB	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	159	CG	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	160	CD	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	161	CE	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	162	CF	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	163	CGA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	164	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	165	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	166	CA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	167	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	168	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	169	CB	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	170	CG	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	171	CD	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	172	CE	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	173	CF	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	174	CGA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	175	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	176	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	177	CA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	178	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	179	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	180	CB	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	181	CG	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	182	CD	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	183	CE	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	184	CF	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	185	CGA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	186	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	187	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	188	CA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	189	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	190	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	191	CB	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	192	CG	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	193	CD	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	194	CE	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	195	CF	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	196	CGA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	197	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	198	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	199	CA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	200	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	201	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	202	CB	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	203	CG	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	204	CD	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	205	CE	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	206	CF	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	207	CGA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	208	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	209	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	210	CA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	211	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	212	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	213	CB	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	214	CG	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	215	CD	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	216	CE	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	217	CF	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	218	CGA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	219	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	220	O	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	221	CA	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C
ATOM	222	C	PRO A	22	-10.097	-2.388	-8.181	1.00	20.38	6	A	C